SPECTRAL STUDIES IN HIGHLY IONISED ATOMS OF YTTRIUM, ZIRCONIUM, NIOBIUM AND MOLYBDENUM

Lund 1981

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Document name
DOCTORAL DISSERTATION

Date of issue
April 3, 1981

CODEN:

Author(s)
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Sponsoring organization

Title and subtitle

Spectral Studies in Highly Ionised Atoms of Yttrium, Zirconium, Niobium and Molybdenum

Abstract

A parametric study of the experimental data available on p^2, p^3 and p^4 configurations is performed on the basis of the Intermediate Coupling Theory. It is concluded that the LS and LS-like couplings are applicable only to well-defined portions at the beginning of the sequences involved, with n = 2 and 3. The Z-dependence of the intervals of $4s^24p^4$ is studied.

Transitions 4p-5d, 6d and 4p-6s, 7s are identified in the Br I - like spectra of Y V, Zr VI, Nb VII and Mo VIII for the first time. Energy levels of the higher excited configurations are determined and the ionisation potentials of these spectra evaluated; that of Sr IV is improved upon.

The spectra Y VI - VIII, Zr VII - IX, Nb VIII - X and Mo IX - XI, belonging to the sequences of Se I, As I, and Ge I are studied for the first time. Transitions 4p - 5s, 4d are identified to establish all the levels of the 4p and 5s configurations, together with 23 $4p^34d$, 19 $4p^24d$, 11 4p4d and 2 $4s4p^4$ levels in each of the four sequence members concerned.

In Mo IX, transitions 4p - 5d, 6d and 4p - 6s, 7s are also worked out to determine the energy levels involved an the series limit of the spectrum.

These spectra were produced in a sliding spark or an open spark source in vacuum and recorded in the grazing incidence region (50 - 430 Å).

Key words

Spectra of highly ionised atoms, configuration interaction

Classification system and/or index terms (if any)

Supplementary bibliographical information

Language
English

ISSN and key title

ISBN

Recipient's notes

Number of pages
76

Price

Security classification

Distribution by (name and address)

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DOKUMENTDATABLAD enl SIS 61 41 21

SPECTRAL STUDIES IN HIGHLY IONISED ATOMS OF YTTRIUM, ZIRCONIUM, NIOBIUM AND MOLYBDEN

AVHANDLING FÖR FILOSOFIE DOKTORSEXAMEN VID MATEMATISK-NATURVETENSKAPLIGA FAKULTETEN VID UNIVERSITETET I LUND. AVHANDLINGEN KOMMER ATT FÖRSVARAS VID EN OFFENTLIG DISPUTATION A FYSISKA INSTITUTIONENS FÖRELÄSNINGSSAL B ONSDAGEN DEN 29 APRIL 1981 KL 10.15

AV

MIRZA SAID-UZ-ZAFAR CHAGHTAI

M SC, MLM

AVHANDLINGEN FÖRSVARAS PÅ ENGELSKA

DEDICATION

This collection of papers I humbly place at the feet of my Great Master

Professor BENGT EDLÉN

M. S. Chaghtai

M.S.Z. Chaghtai
Aligarh
1st January 1981

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SPECTRAL STUDIES IN HIGHLY IONISED ATOMS OF YTTRIUM ZIRCONIUM, NIOBIUM AND MOLYBDENUM

Mirza Said-uz-Zafar Chaghtai

Introduction

Spectral studies of ionised atoms go back to Pickering's observing the He II lines in the spectrum of ζ-puppis star in 1897. After the Bohr-Summerfeld theory of atoms was propounded Millikan, Bowen, Fowler, Paschen, Gibbs and White were prompted to study in the laboratory, one, two or many times ionized atoms-isoelectronic with neutral Na, K, Ca, Sc and Ti (1).

Systematic work on precision spectrography of ionised atoms was taken up by Edlén in late twenties at Uppsala (2). He established with great painstaking a reliable reference system of spectral lines 160 - 1371 Å by comparing persistent lines of C II, III, IV, OII, III, IV, V and Al IV, V, VI in their higher spectral orders with Fe secondary standards available down to near ultraviolet region, and published a complete chart of strong C, N, O etc. lines recorded and measured in vacuum U.V. This laid the foundation of Edlén school.

Importance of Edlén's accurate measurements and analyses of the 1st, 2nd, 3rd and higher spectra of Li, Be, B, C, N, O and other atoms was fully realised in 1942 on his identifying all the important lines of the solar corona (3) and the stunning conclusion that there exist dynamic temperatures of order two million degree centigrade even outside the core of the stars. Edlén's life-long work on the isoelectronic and other regularities in Atomic Spectra(4) is responsible for great progress in the subject.

After the second world war, rockets and then artificial satellites could be used to record soft UV- and X-radiation about 50 km above the earth's surface. Coming from our sun, other stars and the outer space, it gets absorbed in the atmosphere before reaching us. Edlén has vividly described these recordings upto 1968 (5). As regards solar spectrum, we can particularly remember efforts of the groups of Tousey (NRL 1946 etc.), Friedman (NRL 1963 etc.) and Neupert (Goldard Space Flight Center 1967 etc.) reaching wave-lengths shorter than 1 Å.

This new wealth of spectral data, which is still pouring in, is crucially important to astrophysical and space studies. Identification of the solar spectrum lying below 220 Å presented a major challenge. That was met by producing a hot plasma spectrum first at the Zeta machine of Harwell (6) and then the Θ-pinch at Culham (7). The strong lines 165 - 220 Å came out to belong to Fe VIII-XIV and the weaker ones at shorter wave-lengths to Ni X-XIV.

Ionisations go on increasing as we proceed to shorter wavelengths. About 15 Å, Fe XVII, VIII and O VII, VIII etc. dominate; and by the time 1 Å is reached, helium I- and hydrogen I-like 2- and 1-e spectra of Fe and heavier atoms are the ones to contribute.

Laser-produced plasma (8) and the improved versions of the old condensed spark (9), sliding spark (10,11) and triggered spark (12) have been used to great advantage for producing spectra from highly ionised atoms. But the work of interpretering these spectra advanced mainly because the advent of computers after 1950 made ab initio calculations of complicated spectra possible with ever-increasing refinements. Hartree's monograph on 'Calculation of Atomic Spectra'(13) was followed by a series of computer programs develloped, revised and improved upon by a number of workers. Froese-Fischer (14) and Hibbert (15) have reviewed the subject in detail recently.

For the practical help brought to most of work on the analysis of atomic spectra in the last fifteen years or so, Cowan deserves a special mention (16). First he developped his adapted Hartree (HX) calculations method, simplifying the Hartree-Fock formalism by substituting Fermi-Thomas approximation for self-energy. A lot of computer time could be saved thus against a small loss in accuracy of results. Second, he introduced the procedure of scaling the Hartree-Slater, parameters F^k, G^k, ζ_{np} and R^k by fitting them to the experimental data of a reliably analysed analogous spectrum. This permitted predicting structure of heavy atoms and ions with only a few per cent error in favourable cases. The theory would otherwise depart from the experiment by large amounts due to relativistic effects, which are unaccountable in the usual HF formalism despite prescribed corrections.

Development of short wave-length lasers (17) requires detailed Physics of the structure of multiply ionised atoms. At high temperature ($T \sim 10^5$K), radiation pyrometry is the only means of determining the existing dynamic conditions, and this depends on accurate spectroscopic knowledge of the atoms involved. Spectrography of highly ionised atoms is, therefore, of basic use to plasma diagnostics (18) and studies in controlled nuclear fussion (19). From Tokamak (plasma) machines, XUV radiation of highly ionised Mo atoms has been recorded and interpretted recently(20).

By 1960, back pumping from nuclear to atomic physics gave birth to the remarkable field of studies called Beam-Foil Spectroscopy (BFS)(21). Life time of an enormous number of excited levels, not only of the ionised and highly ionised atoms to which the technique is particularly applicable, but also of neutral atoms were directly measured, introducing notable improvements in the theoretical and experimental techniques involved (22). BFS

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provided copious data on multiply excited levels, improving upon the theory of the autoionised states (23). Studies of spectral terms involving high n and large l values added to the understanding of hydrogenic states (24), whereas asymmetries observed in BF radiation tell us a lot more of the surface effects of the foil used and the nuclear effects of its atoms than what we understand so far (25).

Summary

The work on the analyses of atomic spectra, that we are presenting herewith, was started in Paris/Orsay in 1963 and the first results published in 1969-70 (26) were communicated from Lund. All the spectra we have used thereafter have been recorded in the Physics Department of Lund University, on the 5-m grazing incidence spectrograph as regards the present work, that consists of the following papers:

1. A theoretical study of the np^k configurations.
   K. Rahimullah and M.S.Z. Chaghtai, J. Quart.Spectrosc. Radiat. Transfer 16 105-12(1976).
2. Coupling conditions and level structure of the p^4 configurations
   M.S.Z. Chaghtai and K. Rahimullah, Nuovo Cimento 17A 162-70 (1973).
3. Term Analysis of Y V
   Z. Ali, M.S.Z. Chaghtai and S.P. Singh, J. Phys. B,185-93(1975)
4. Transitions 4p-5d, 6d and 4p-6s, 7s in Zr VI and Nb VII
   M.S.Z. Chaghtai, K. Rahimullah and S. Ahmad, J. Phys. B. 7 2121-33 (1974).
5. Observation and Classification of 4p-5d, 6d and 4p-6s, 7s Transitions in Mo VIII, M.S.Z. Chaghtai, S.P. Singh and S. Khatoon J. Phys. B 8 1831-7(1975).
6. 4p-5s Transitions in Y VII, VIII, Zr VIII, IX, Nb IX, X and Mo X, XI.
   K. Rahimullah, M.S.Z. Chaghtai and S. Khatoon
   Physica Scripta 14 221-3(1976).
7. The Transitions 4p-5s in Y VI, Zr VII, Nb VIII and Mo IX
   M.S.Z. Chaghtai, K. Rahimullah and S. Khatoon
   Physica Scripta 14, 281-4 (1976).
8. The 4p-4d Transitions of Y VI, VII, VIII, Zr VII, VIII, IX, Nb VIII, IX, X and Mo IX, X, XI, K. Rahimullah, M.S.Z.Chaghtai and S. Khatoon, Physica Scripta 18 96-106 (1978).
9. The 4p-5d, 6d and 4p-6s, 7s transitions of Mo IX.
   S. Khatoon, M.S.Z. Chaghtai and K. Rahimullah
   Physics Scripta 19 22-24 (1979).

These papers can be arranged in four inter-related groups to describe their contents briefly as under:

A. Theory of the Configurations p^2, p^3 and p^4

Paer 1 and 2 deal with the level structure of p^2, p^3 and p^4 in light of the latest experimental data on these astrophysically important ground configurations and their relation with the intermediate coupling theory of Condon and Shortley as treated by Edlen. First, reduced energy $\epsilon = E/\zeta_{np}$ of all the known levels concerned in the three cases is plotted separately against the parameter $\psi = \zeta_{np}/(5F_2 + \zeta_{np})$; it is concluded that the data separate out in isoelectronic sequences, whose regularity is sensitive enough to judge the accuracy of reported levels. A new diagram (Fig. S1) is enclosed with this summary to give updated picture of our 1973 assessment. $(F_2 - \zeta_{np})$ is then plotted against ψ and it is observed in the three cases that the graphs rise smoothly to a maximum at about $\psi = 0.07$ and become negative for $\psi \gtrsim 0.17$. It is concluded that these points determine limit of validity for LS and LS-like couplings (say IK), beyond which a jj-like situation prevails over major part of the sequences beginning at n = 2, 3, and over the whole sequences beginning at a higher n number.

The Z-dependence of the ground intervals $4s^2 4p^4$ have been studied theoretically for the first time. The known level values are reproduced within 0.02% error by semi-empirical formulae having 3-5 adjustable parameters determined from laboratory observations. Intervals are calculated upto Sb XVIII.

B. Br I-sequence: CONFIGURATIONS 5d,6d,6s, and 7s of Y V, Zr VI Nb VII and Mo VIII

Papers 3-5 deal with the identifications of 4p-5d, 6d and 4p-6s, 7s transitions in the spectra of Y V, Zr VI, Nb VII and Mo VIII. These higher excited configurations are studied for the first time in these spectra permitting experimental evaluation of their ionization potentials as 6.047, 7.770, 9.609 and 11.579 X $10^5 cm^{-1}$. An isoelectronic comparison of the I.P. led to improve the value of Sr IV to 4.462 X 10^5 cm^{-1}.

Theoretical parameters G_1 and ζ_{np} are calculated for the spectra Rb I-Pd XII from the 4p and ^2P levels of $4p^4$ ns configurations on the hypothesis that the ^2S and ^2D terms do not affect them (ref. 4 p.132). E/ζ_{np} is plotted against G_1/ζ_{np}, some notable features discussed and the peculiarity of Rb III pointed out.

Since the publication of paper 5, improvements have taken place in the data on this isoelectronic sequence. Fig. S 2-4 are, therefore included in this summary to up-date the situation of 6s and 5d levels. 6s $(^3P_1)_{3/2}$ and $(^3P_0)_{1/2}$ levels of Y V are revised by us to 446716, 446221, $(^3P_2)_{5/2}$ of Nb VII to 663535 and

$(^1D_2)_{5/2,3/2}$ of Mo VIII to 825900 and 826096 cm^{-1} respectively. Values of Sr IV and revised values of Kr II have been inserted to more aesthetic satisfaction.

It is known that δ vs T plots do not actually converge to the parent levels with increasing n. Indications in this regard in our published Rydberg diagrams are meant to assign the parentages to the extent of term levels.

Misprints detected in these papers may please be corrected as under:

Paper 3 (.... Y V) p 192, last but 3 line. The levels '5p' should be read '5s'

idem p 193, last but 1 line. The ref. should be read: Tech JL 1963 J Res Nat Bur Std 67A 505

Paper 5 (...Mo VIII) p 1837, same as above.

Paper 4 (... Zr VI and Nb VII) p 2124, Table 2, Column 'Classification' 6s and 7s levels:
The parent level is misprinted everywhere $^3P_2$
It should be read:
$^3P_1$ in lines 2,3,9,10,15 and $^3P_0$ in lines 4 and 11.

C. Isoelectronic sequences Se I, As I and Ge I: 4p,4d and 5s levels of Y,VI,VII,VIII, Zr VII,VIII,IX,Nb VIII,IX, X and Mo IX, X, XI.

Papers 6-8 fall in this category. Paper 6 gives an original and almost complete account of the 4p, 5s levels and 4p-5s transitions for seven of these spectra; it improves upon my own earlier work on Nb IX. All the four ground $4p^3$ intervals and the eight $4p^25s$ levels of Y VII, Zr VIII, Nb IX and Mo X are firmly established on the basis of 25, 21, 19 and 18 transitions identified in these As I-like spectra. In Ge I-sequence, all the five $4p^2$ and the four 4p5s levels are determined by identifying 12,10,9 and 12 4p-5s transitions in Y VIII, Zr IX, Nb X and Mo XI.

Paper 7 up-dates our own earlier work on the 4p-5s transition of the Se I-like spectra Y VI, Zr VII, Nb VIII and furnishes a new analysis of Mo IX. This gives the final version on all the four ground intervals of $4p^4$ and the ten levels of $4p^35s$ configurations of these spectra, based on 33, 28, 27 and 25 observed transitions out of the maximum 35 allowed by J-selection rule. The knowledge of the ground intervals is now complete upto the 9th member of this sequence.

Paper 8 comprises studies of 4p-4d transitions in all the twelve spectra concerned. The eight As I- and Ge I-like spectra are analysed for the first time, while our own old work on the four Se I-like spectra is revised. New Cowan calculations are

used in all this work, taking into account the important 4s-4d interactions that displace some levels from their one-configuration position by about 40000 cm^{-1}. Based on 153,152,147 and 165 transitions identified in these spectra, we have determined 23 $4p^3 4d$, 19 $4p^2 4d$, 11 4p4d and 2 4s $4p^4$ levels in each of the four sequence members concerned.

D. Supplementary Analyses

Paper 9 adds analyses of the 4p-5d, 6d and 4p-6s, 7s transitions of Mo IX to our paper 7 and makes it possible to evaluate the series limit of this spectrum to five places, i.e. 1 323 700 ±700 cm^{-1}, with the help of ten smooth ns Rydberg series. All the ten 6s, 7s levels are reported along with 16 5d and 14 6d.

ACKNOWLEDGEMENTS

The kind patronage of Professor B. EDLÉN has made all my work on Atomic Spectra possible from my Paris days(1963) till now; this includes material and moral support of every sort and teaching me the subject! I request him to accept my profoundest and sincerest thanks and expressions of gratitude in this regard.

I am highly indebted to the fraternal collaboration of Dr. J.O. EKBERG in recording spectrograms of my need in Lund.

Dr. R.D. COWAN has been very generous and kind to me over the last twelve years in furnishing his HX and HF calculations concerning my work, involving a lot of computer time and his personal attention to the matter. I thank him for this benevolence sincerely.

I must also remember with thanks on this occasion Prof. Mlle. Y. CAUCHOIS of Paris University, under whose direction I initiated Atomic Spectrography, and Dr. P. JAEGLÉ, who introduced me to grating spectrograph techniques.

I am highly indebted to and appreciative of my research students at Aligarh, many of them coather research papers with me, specially Dr. Zahid Ali and Dr.Mrs. Sabra Khatoon(Mushir) whose deligence established me at Aligarh as an Atomic Researcher and Dr. Khan RAHIMULLAH who has been the strength of my right hand in the laboratory all these years and who will remain so as a colleague for many many years to come.

I will fail in my duties if I do not record my gratitude and appreciation for the staff of the laboratoire de Chimie Physique Paris/Orsay and the Departments of Physics of Lund and Aligarh Muslim Universities for their help and assistance on innumerable occasions.

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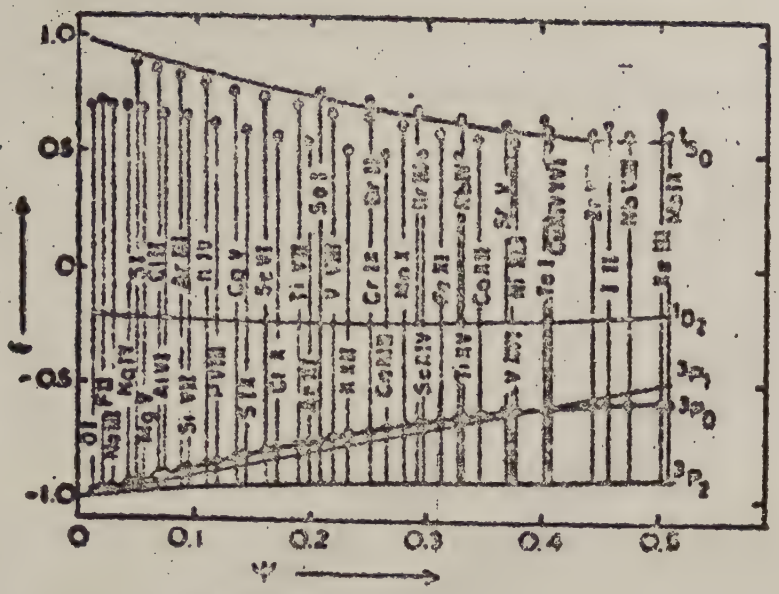

FIG. S_1 p^4 INTERVALS.

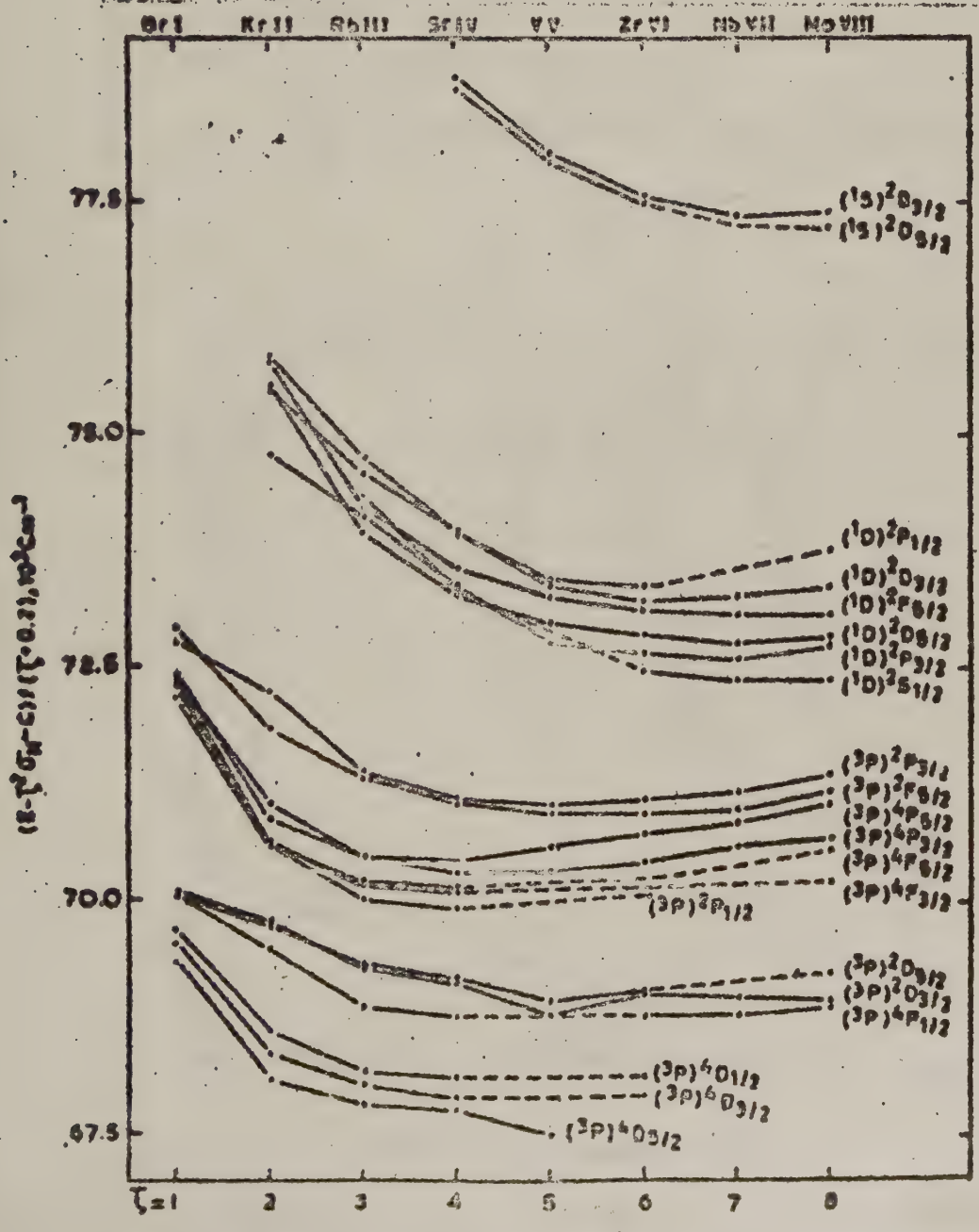

FIG. S_2 $4p^4\,5d$ LEVELS OF BrI SEQUENCE. $\sigma_H = 2469\,cm^{-1}$
C IS c.g. OF $4p^3\,{}^2P$.

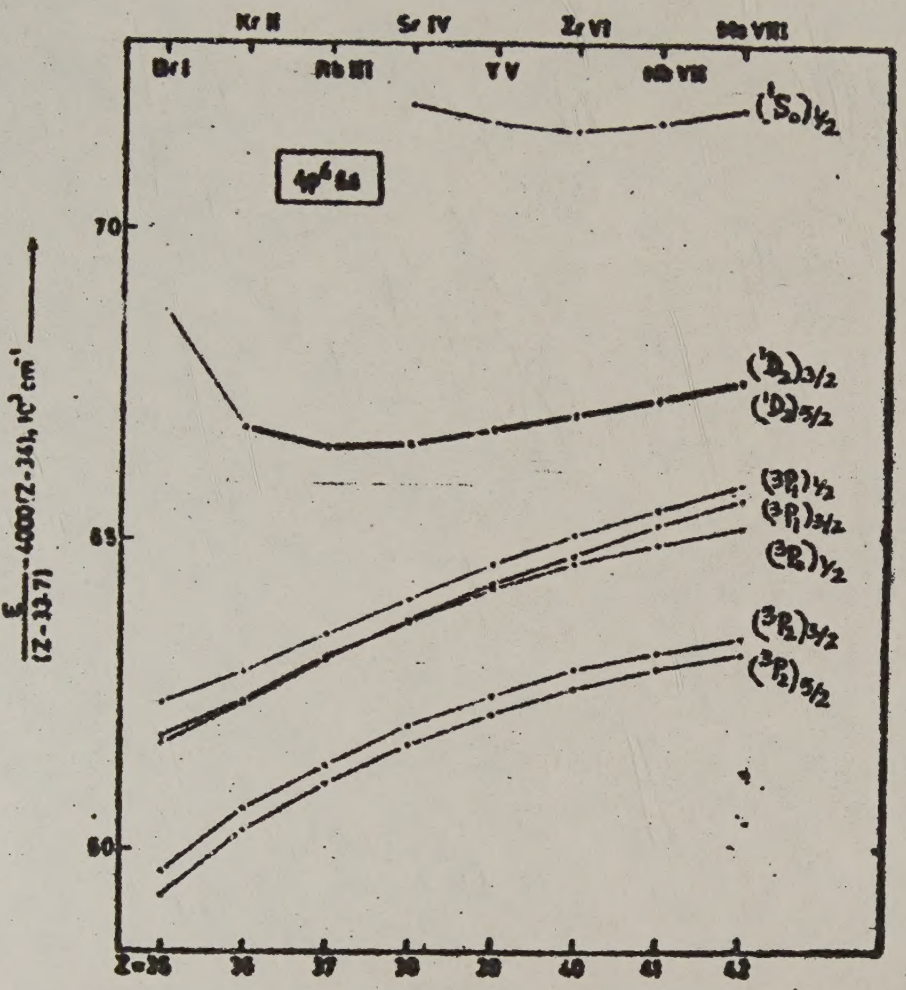

FIG. S3 Br I-like 4s levels